



Numerical analysis of elastic and elastoplastic behavior of interpenetrating phase composites



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ABSTRACT

A routine is compiled to describe the spatial distributions of interpenetrating phases by solving the phase field equation. And a 3D random finite element (FE) model based on the phase field method is presented which can characterize the realistic microstructure of the interpenetrating phase composite (IPC) for the first time. Compared with the previous models, the present model is easier to generate at a low cost. The statistical criterion has been employed to determine the critical size of the 3D random FE model. The sample capacity has also been discussed. In addition, the cross-cubic model and the tetrakaidecahedron model are also conducted by finite element method (FEM) for comparison. Furthermore, the Young's modulus and elastoplastic properties of IPC are predicted by FE models and theoretical methods, and the results of the 3D random FE model accord well with experimental data.

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1. Introduction

The interpenetrating phase composites (IPCs), also called co-continuous or bicontinuous composites are advanced engineering materials which consist of two pure phase materials. Each phase contributes its own properties to the multifunctional characteristics of the whole structure. If either of the two phases were removed from such a composite, the remaining constituent would form an open-cell foam, which alone can still bear loads. As constituents of composite are interconnected in 3D space and twine in all directions, the interface-to-volume (interface denotes interface/surface between two phases) ratio is pretty high. Hence, IPCs possess unique mechanical properties and physical properties which are different from and even superior to the conventional fiber or particle-reinforced materials. There are various IPCs composed of different constituents, for example ceramic-metal [1], interpenetrating polymer network [2] and metal/ceramic foam base IPC [3–6].

It is a challenge to study the mechanical properties of IPCs for their complicated microstructures. Previous work on this subject can be broadly classified into three categories, namely theoretical methods [7–9], experimental measurements [10,11] and computational simulations [12–22]. Because of the complex microstructure of the IPCs, an analytical method can hardly estimate the mechanical properties precisely. And experiment tests are inconvenient and costly. Hence, computational simulation methods are always

employed and documented in literature. With 2D mesoscopic model using the Voronoi tessellation technique, Wang et al. [12] performed FE analysis on the representative volume element to study the mechanical properties of IPC. Singh et al. [13,14] presented a 2D unit cell model to numerically simulate the elastoplastic behavior of IPC using the element free Galerkin method (EFGM). Senthil et al. [15,16] used the random morphology description functions (RMDFs) to generate a so-called realistic random microstructure (2D) for computational analyses. Chen et al. [17] developed a routine for creating 2D FE models characterizing the microstructure observed in a SEM using a backscattering detector. However, a 2D model can hardly characterize IPCs exactly, whose constituents are interconnected in 3D space instead of scatter. Tuchinskii [9] presented a skeletal structure to estimate the elastic constants of pseudoalloys by theoretical analysis method. Feng et al. [7,8] presented a micromechanical model to estimate the effective elastic moduli of IPC by theoretical analysis method and finite element method. Furthermore, the elastoplastic behavior was derived via a step-by-step analysis of the unit cell. Jhaver and Tippur [3] presented a Kelvin cell based 3D elastoplastic finite element model capable of capturing both linear and nonlinear characteristics of the IPC foams. Nevertheless, these micromechanical models are far different from the realistic microstructure of IPC. To approach the realistic microstructure, Alveen et al. [18] presented a representative finite volume (FV) microstructure using Voronoi tessellation to synthetically represent the microstructure of a two phase ceramic composite. Poniznik et al. [19] established a random voxel model by FEM to estimate the effective elastic properties of metal-ceramic interpenetrating phase composites, and a

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realistic microstructure FE model was introduced by contrast. These two FE models were much more approximated to the realistic structure of the materials compared to Tuchinskii's model [9], Feng's model [7,8] and Jhaver's model [3]. Basista et al. [20] developed a computational model to determine the Young modulus of IPC using 3D images of realistic material microstructure obtained from X-ray tomography. Nonetheless, obtaining the FE model based on a realistic microstructure is complex and expensive, which demands equipment severely. Except mesh-free method and FEM, molecular dynamics simulations (MDs) are also employed to study nano-IPCs. Yang and Lu [21] investigated the mechanical behavior of co-continuous Cu/SiC nanocomposites by MDs. They concluded that both the volume fraction (VF) of the components and temperature could affect the mechanical properties. Sun et al. [22] summarized four models to discuss the tensile property of IPC by MDs. It was concluded that the connectivity of microstructure in a certain direction strongly affects the effective Young's modulus and strengths of nanocomposites in this direction.

The interpenetrating metal-ceramic and pseudo-alloy are advanced engineering materials which have extensive applications. The fabrication of these IPCs always involves two steps, one of which is to prepare an interconnected porous structure, and the other is to infiltrate the molten phase into the porous structure [23,24]. In order to better predict material behavior, it is a key problem to establish a model which can describe the realistic microstructure of porous structure with co-continuous structure. Chen and Shen [25] characterized a co-continuous structure via solving the phase field equation and obtained realistic morphology. Inspired by the previous work, a realistic morphology is introduced into FEM and a random 3D FE model is presented to characterize the IPCs based on the phase field method for the first time.

The objective of this paper is to study the mechanical behavior of IPCs and the organization is as follows. First, the FE models (random, cross-cubic and tetrakaidecahedron models) are presented in detail. Next, the statistical and error analyses are introduced to determine the optimized random model parameters. Afterward, the optimized model is employed to predict the elastic and elastoplastic properties of IPCs. The influences of the constituents' material parameters on the mechanical behaviors are also analyzed.

2. Models

2.1. Random model

IPCs have a complicated bicontinuous microstructure (Fig. 1) as their processing methods include direct porous structure and another phase infiltration into the matrix. To better mimic this

process, a random porous model should be built at first, and then fill the porous model with another phase to obtain the whole IPC model. The phase field method has been usually employed to characterize the bicontinuous structures [22,26–29]. Sun et al. [22] established a bicontinuous structure based on the phase field method and MDs was implemented to obtain the mechanical behaviors of nano-IPC. Crowson et al. [26,27] probed the dominant mechanisms for the geometric relaxation of bicontinuous nanoporous metal based on the phase field method. Farkas et al. [28] and Sun et al. [29] studied the mechanical properties of nanoporous gold with bicontinuous structure based on the phase field method. As Section 1 mentioned, the existing FE models are either too simple to characterize the IPCs, or so expensive to obtain based on X-ray CT scan. Consequently, we utilize the phase field method to obtain the model information and implement FEM to establish model.

In the phase field method, the pattern evolution can be described by the Cahn–Hilliard equation [30]. The Cahn–Hilliard equation has a rather broad range of application. It can serve as a good model for the dynamics in a sufficiently accurate fashion so that many of the various features of the resultant pattern formation evolution during phase separation can be explained and predicted. As mentioned in Ref. [30], this pattern formation is referred to as the microstructure of the material in materials science. Consequently, a random bicontinuous structure pattern can be obtained by the following Cahn–Hilliard equation.

$$u_t = \nabla \cdot \left\{ M(u) \nabla \left[\frac{df(u)}{du} - \frac{\epsilon^2}{2} \Delta u \right] \right\}, \quad (1)$$

where $u(x,y,z,t)$ is the difference in concentration of the two phases, t represents the evolutionary time, u_t denotes the partial time derivative of u , $f(u)$ is a free energy function, $M(u)$ is a “mobility” coefficient, $0 > \epsilon^2 \ll 1$ is a “coefficient of gradient energy”, ϵ denotes the width of transition region between the two phases. In this study, we simply adopt the double-well potential function $f(u) = \frac{1}{4}(u^2 - 1)^2$, and consider $M(u)$ as a constant coefficient 1 and set $\epsilon = 0.01$ which does not influence the results qualitatively. We adopt the central difference method to discretize Eq. (1). A set of initial values are randomly generated near zero, and periodic boundary conditions are adopted in all three directions. The size of computational domain determines model size, which can be adjusted as needed.

We set a cutoff value u_0 to distinguish different phases. If $u \geq u_0$, the coordinate position is occupied by one phase, otherwise the coordinate position is the other phase. We can change the value of u_0 to obtain various VFs of constituents. Indeed, different random models can be obtained at different evolution time.

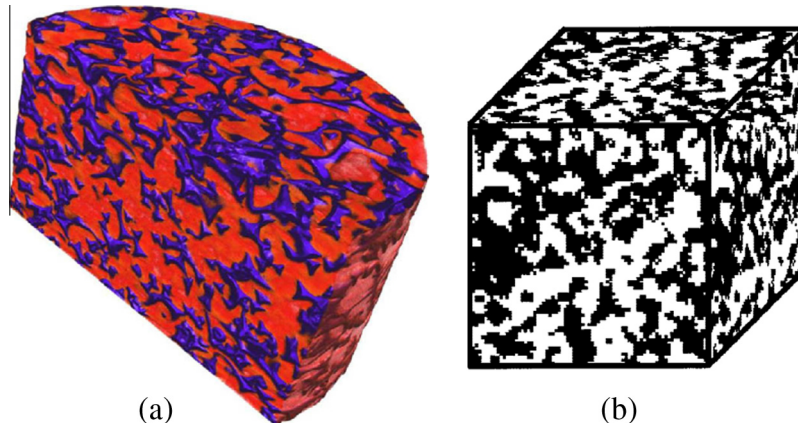


Fig. 1. (a) Microstructure of Al_2O_3 -Cu composite, X-ray CT scan [19]. Reused with permission from ref. [19]. Copyright 2008 Elsevier. (b) Schematic of an interpenetrating two-phase composite [38]. Reused with permission from ref. [38]. Copyright 2004 John Wiley and Sons.

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